

K-13870-M1

Table S1: ^{15}N and ^1H Resonance Assignments for CheA₁₋₁₃₄ at pH 6.3 and 30 °C^a

residue	amide N	amide H	α H	others
M1				
S2				
M3	122.9	8.46	4.53	2.75, 2.59, 2.00
D4	123.3	8.55	4.69	2.73, 2.60
	122.9	8.46	4.69	2.73, 2.60
I5	122.2	8.16	4.23	1.93, 0.94, 1.25
	122.1	8.22	4.23	1.93, 0.94, 1.25
S6	122.1	8.28	4.42	H β (3.85)
D7	122.9	8.26	4.54	H β (2.55, 2.60)
F8	120.3	7.97	4.52	H β (3.09), H δ (7.21), H ϵ (7.35)
Y9	119.4	7.72	3.71	H β (2.82, 2.58), H δ (6.79), H ϵ (6.85)
Q10	118.6	7.94	3.97	2.23, 2.14, H γ (2.47), N ϵ^2 (115.4), H ϵ^2 (6.92, 7.89)
T11	113.1	7.91	4.28	H β (4.13), H γ (1.31)
F12	122.6	7.53	4.51	H β (3.23, 2.56), H δ (7.09), H ϵ (7.22)
F13	119.1	8.31	4.02	H β (3.30), H δ (7.17), H ϵ (7.25)
D14	118.5	8.29	4.39	H β (2.79)
E15	122.4	8.06	4.06	H β (2.06), H γ (2.43, 2.19)
A16	122.9	9.21	3.82	H β (0.93)
D17	118.9	8.32	4.44	H β (2.90, 2.59)
E18	121.1	7.44	4.13	2.22, 2.47
L19	122.5	8.69	4.21	1.99, 1.32, 0.96
L20	121.5	8.92	4.11	2.08, 0.93
A21	123.0	7.61	4.26	H β (1.52)
D22	121.4	8.33	4.41	H β (2.84)
M23	121.1	8.94	3.95	2.65, 2.39, 2.27, H γ (2.89)
E24	119.3	8.21	3.78	2.35, 2.17, 1.93
Q25	116.0	7.92	3.91	2.40, 2.09, N ϵ^2 (113.2), H ϵ^2 (6.78, 7.47)
H26	114.8	7.86	4.41	H β (3.06)
L27	121.1	8.57	3.96	H β (2.30, 1.86), H γ (1.28), H δ (0.78, 1.09)
L28	115.8	7.92	4.15	1.89, 1.50, H β (0.92)
V29	109.6	7.07	4.53	H β (2.42), H γ (0.97)
L30	125.5	7.20	4.19	1.78, 1.57, H δ (0.95, 0.82)
Q31	126.6	8.89	4.79	H β (2.04, 2.15), H γ (2.45)
P32				
E33	114.5	8.81	4.22	H β (2.00), H γ (2.30, 2.08)
A34	121.8	7.43	4.63	H β (1.23)
P35				
D36	125.8	8.20	4.59	H β (2.71)
A37	130.8	8.99	3.96	H β (1.51)
E38	118.0	8.39	4.26	2.35, 2.15
Q39	121.2	8.14	3.98	2.22, 2.14, H γ (2.52), N ϵ^2 (112.2), H ϵ^2 (6.96, 7.73)
L40	118.0	8.00	4.02	1.86, 1.36, 1.67, 0.82
N41	118.4	8.58	4.43	H β (2.98, 2.78), N δ^2 (112.5), H δ^2 (6.91, 7.59)
A42	123.4	7.89	4.03	H β (1.05)
I43	120.8	7.85	3.59	2.01, 1.85, 0.89, 0.81
F44	120.2	8.45	3.88	H β (3.29, 2.87*), H δ (7.05), H ϵ (6.81)
R45	119.1	8.85	3.79	1.97, 1.86, 1.62, 0.94, H β (3.25)
A46	122.3	7.57	4.20	H β (1.58)
A47	120.1	7.96	3.73	H β (1.23)
H48	116.9	8.92	4.26	H β (2.99, 2.40)
S49	117.4	8.36	4.24	H β (3.92)
I50	124.6	8.18	3.84	1.96, 1.42, 1.39, 1.05, 0.81
K51	121.6	8.55	3.69	1.81, 1.04
G52	105.6	7.82	3.85, 3.63	
G53	110.8	7.93	3.63, 3.60	
A54	123.3	8.89	3.78	H β (1.56)
G55	103.7	8.06	3.82, 3.64	
T56	120.6	7.60	3.56	H γ (0.37)
F57	116.5	6.90	4.24	H β (2.31, 1.19), H δ (6.60), H ϵ (6.86)
G58	107.3	7.21	3.94, 3.78	
F59	122.4	8.14	4.86	H β (3.76, 2.74), H δ (6.53), H ϵ (6.94)
S60	119.8	8.05	4.08	H β (3.94)
V61	122.2	7.91	3.36	H β (1.75), H γ (0.54, 0.17)
L62	122.5	6.78	4.95	1.97, 1.77, 1.57, 1.30*, 1.19*
Q63	122.8	8.65	3.67	2.33, 1.65, N ϵ^2 (110.2), H ϵ^2 (6.79, 7.17)
E64	119.0	8.39	4.41	H β (2.19), H γ (2.49, 2.26)
T65	117.1	8.17	3.92	H β (4.44), H γ (1.23)
T66	113.2	8.21	3.85	H β (4.05), H γ (1.34)
H67	122.8	8.63	4.31	H β (3.25)
L68	118.4	7.91	3.94	2.09, 1.38, 1.03, 0.82
M69	119.5	7.81	4.00	2.18, 2.05
E70	121.4	9.40	3.76	H β (2.05), H γ (2.24, 2.35)

N71	117.8	8.05	4.57	H β (2.84), N ϵ^2 (109.9), H ϵ^2 (6.39, 7.52)
L72	120.1	7.30	4.20	2.15, 1.58, 1.98, H δ^1 (1.13), H δ^2 (0.89)
L73	120.1	8.58	3.96	2.21, 1.38, H δ^1 (0.40), H δ^2 (0.66*)
D74	120.5	8.84	4.29	H β (2.87)
E75	117.7	7.67	3.97	2.57, 2.36
A76	121.7	8.41	4.52	H β (1.58)
R77	120.8	8.88	4.08	2.03, 1.66, H δ (3.20)
R78	117.7	7.65	4.33	2.03, 1.72, 1.58, H δ (3.10)
G79	107.9	7.83	4.19, 3.91	
E80	118.5	8.02	4.29	2.21, 1.84
M81	117.2	7.00	4.55	1.92, 1.63, 2.37, 2.26
Q82	126.2	8.66	4.37	H β (2.09, 1.93), H γ (2.40), N ϵ^2 (113.8), H ϵ^2 (6.82, 7.62)
L83	122.5	8.91	4.33	2.07, 1.87, 2.38, H δ^1 (1.11), H δ^2 (0.85)
N84	112.6	6.72	4.58	H β (3.21, 3.04), N δ^2 (113.8), H δ^2 (7.01, 7.48)
T85	114.8	8.78	3.85	H β (4.12), H γ (1.23)
D86	122.5	7.96	4.43	H β (2.74, 2.57)
I87	122.9	8.37	3.39	2.01, 1.78*, 1.35, 0.82, 0.23
I88	120.2	7.78	3.54	2.00, 1.14, 1.07, 0.77
N89	118.7	8.45	4.63	H β (3.02, 2.89), N δ^2 (112.1), H δ^2 (6.81, 7.74)
L90	124.9	7.97	4.44	1.84, 1.61, 0.86, 0.78
F91	123.6	8.86	3.73	H β (3.12, 2.26), H δ (7.00), H ϵ (7.05)
L92	123.3	8.74	4.07	2.13, 1.71, 0.99
E93	122.0	8.46	4.18	2.34, 2.15, H γ (2.55)
T94	118.1	8.67	3.82	H β (4.32), 1.24
K95	124.3	8.35	4.07	1.88, 2.18, 1.23
D96	121.4	8.00	4.53	H β (2.99, 2.76)
I97	124.2	8.37	3.90	2.02, 1.02, 1.23, 0.70
M98	122.6	9.20	4.09	2.39
Q99	119.4	8.39	4.42	2.50, 2.26, N ϵ^2 (115.8), H ϵ^2 (7.19, 7.45)
E100	119.9	7.84	4.07	2.53, 2.27, 2.12
Q101	122.3	8.62	3.69	2.71, N ϵ^2 (102.4), H ϵ^2 (6.24, 6.82)
L102	119.9	8.60	4.00	2.00, 1.60, 0.95
D103	118.5	8.61	4.10	H β (2.69, 2.50)
A104	124.8	7.71	3.98	H β (0.98)
Y105	119.4	7.85	4.37	H β (2.65, 2.61), H δ (6.96), H ϵ (6.71)
K106	121.1	8.40	3.36	1.54
Q107	116.2	7.27	4.48	2.35, 1.84, N ϵ^2 (110.1), H ϵ^2 (6.72, 7.21)
S108	113.5	8.17	4.18	
Q109	118.4	8.17	4.55	2.29, 2.00, 1.64, N ϵ^2 (112.2), H ϵ^2 (6.77, 7.31)
E110	120.9	8.29	4.52	2.36, 1.98, 1.84
P111				
D112	122.5	8.87	4.40	H β (2.71)
A113	133.0	8.84	4.21	H β (1.55)
A114	121.9	8.33	4.25	H β (1.50)
S115	116.5	8.39	4.42	H β (3.98)
F116	122.7	7.30	4.49	H β (3.19), H δ (7.26), H ϵ (7.37), H ζ (7.32)
D117	121.1	8.42	4.09	H β (2.76, 2.68)
Y118	119.1	8.03	4.21	H β (3.31, 3.12), H δ (7.10), H ϵ (6.77)
I119	122.7	8.40	3.85	1.96*, 1.30, 0.89*, 1.02*
C120	121.1	8.14	4.00	H β (2.66, 2.22)
Q121	118.6	7.67	3.97	2.08, 2.31, 2.48
A122	122.9	7.73	3.99	H β (1.20)
L123	118.4	8.53	4.05	1.95, 1.26, 0.89, 0.99*
R124	120.2	8.41	4.00	1.91, 1.59, 1.81, 3.16
Q125	119.2	8.09	4.01	2.19, 2.07, 2.41
L126	119.3	7.49	4.16	1.72, 1.63, 0.86
A127	120.7	7.52	4.10	H β (1.48)
L128	119.5	7.79	4.16	1.79, 1.61, 0.86*
E129	120.4	8.15	4.13	H β (2.07, 2.12), H γ (2.26, 2.41)
A130	123.4	8.15	4.29	H β (1.43)
K131	118.6	7.82	4.36	2.99, 1.94, 1.83, 1.67, 1.50
G132	109.5	8.13	3.95, 4.05	
E133	121.3	8.27	4.41	2.25, 2.10, 1.89,
T134	120.9	7.81	4.18	H γ (1.13)

^a ¹H chemical shifts are relative to DSS. ¹⁵N chemical shifts are relative to ¹⁵NH₃. Chemical shift values indicated by asterisks (*) were obtained from a 3D ¹⁵N-edited NOESY.

K-13870-M3

Table S2

residue	T ₁ (sec)	T ₂ (sec)	NOE	τ_m (ns)	S ²	τ_e (ps)	error (%)
4	0.7857	0.2498		5.51			
4	0.0451	0.0229					
5	0.6543	0.2844		4.19			
5	0.0306	0.0302					
6	1.8723	0.4323	-3.966	6.94	0.163	0.8264E+02	
6	0.2493	0.0686					33.55
7	0.5533	0.1678	0.467	5.71	0.518	0.1930E+04	
7	0.0219	0.0104					33.63
9	0.5428	0.1180	0.736	7.23	0.808	0.4536E+02	
9	0.0207	0.0052					11.14
11	0.5256	0.1098	0.765	7.42	0.853	0.4146E+02	
11	0.0197	0.0044					8.86
12	0.5563	0.1057	0.738	7.89	0.843	0.3437E+02	
12	0.0221	0.0043					2.15
14	0.5324	0.0980	0.806	8.06	0.904	0.8086E-07	
14	0.0201	0.0035					0.86
15	0.5343	0.1053	0.789	7.71	0.866	0.2183E+02	
15	0.0203	0.0041					5.29
16	0.5467	0.0978	0.747	8.20	0.888	0.3136E+02	
16	0.0213	0.0035					1.84
17	0.5366	0.0861	0.870	8.77	0.963	0.4249E-05	
17	0.0205	0.0027					9.97
18	0.5248	0.0989	0.802	7.93	0.904	0.9125E+01	
18	0.0197	0.0036					2.45
19	0.5090	0.0988	0.799	7.79	0.918	0.2364E+02	
19	0.0183	0.0037					4.34
20	0.5808	0.0898	0.800	8.98	0.912	0.3988E-05	
20	0.0245	0.0030					11.48
21	0.5574	0.0942	0.872	8.50	0.900	0.3153E-05	
21	0.0219	0.0033					6.82
22	0.5386	0.0961	0.854	8.21	0.905	0.7826E-05	
22	0.0206	0.0034					3.41
23	0.5548	0.0965	0.808	8.35	0.892	0.2879E-07	
23	0.0219	0.0035					3.21
24	0.5764	0.0927	0.864	8.76	0.895	0.2320E-05	
24	0.0238	0.0032					9.70
25	0.5505	0.0937	0.766	8.46	0.909	0.1094E+02	
25	0.0217	0.0032					4.95
26	0.5459	0.0960	0.841	8.29	0.901	0.9753E-05	
26	0.0213	0.0034					3.47
27	0.5749	0.0865	0.801	9.12	0.937	0.9384E-06	
27	0.0238	0.0027					13.33
28	0.5414	0.0903	0.740	8.57	0.933	0.3754E+02	
28	0.0208	0.0031					6.62
29	0.5660	0.1099	0.737	7.78	0.819	0.3233E+02	
29	0.0231	0.0045					3.58
30	0.5701	0.1179	0.833	7.47	0.798	0.5461E+01	
30	0.0236	0.0054					9.10
31	0.5143	0.1229	0.685	6.79	0.743	0.1630E+04	
31	0.0187	0.0055					18.93
33	0.5434	0.1246	0.635	6.98	0.776	0.7575E+02	
33	0.0209	0.0058					13.21
34	0.6290	0.1295	0.632	7.50	0.705	0.4294E+02	
34	0.0282	0.0062					6.04
36	0.6052	0.1442	0.598	6.80	0.681	0.5535E+02	
36	0.0262	0.0079					15.22

K-13870-m4

37	0.5198	0.0925	0.800	8.23	0.941	0.7490E-04	
37	0.0191	0.0034					1.51
38	0.5353	0.1098	0.727	7.51	0.841	0.5155E+02	
38	0.0201	0.0045					7.13
39	0.5670	0.1066	0.788	7.95	0.837	0.1047E+02	
39	0.0231	0.0042					2.09
40	0.5294	0.1002	0.671	7.91	0.880	0.9292E+02	
40	0.0199	0.0038					0.93
42	0.5123	0.0976	0.764	7.88	0.917	0.4914E+02	
42	0.0186	0.0036					2.65
43	0.5346	0.1004	0.789	7.95	0.888	0.1540E+02	
43	0.0206	0.0038					2.00
44	0.5262	0.1008	0.710	7.85	0.884	0.7109E+02	
44	0.0195	0.0038					2.29
45	0.4983	0.0991	0.829	7.67	0.930	0.5507E+01	
45	0.0179	0.0036					6.40
46	0.5148	0.0983	0.773	7.87	0.912	0.3856E+02	
46	0.0186	0.0035					2.91
47	0.5376	0.1065	0.760	7.69	0.856	0.3490E+02	
47	0.0207	0.0041					5.20
48	0.5222	0.0972	0.774	8.00	0.912	0.2952E+02	
48	0.0196	0.0035					1.19
49	0.5064	0.0963	0.718	7.89	0.923	0.1052E+03	
49	0.0186	0.0034					1.89
50	0.5325	0.0904	0.884	8.48	0.940	0.2005E-06	
50	0.0200	0.0029					7.01
51	0.4992	0.0960	0.766	7.83	0.936	0.6842E+02	
51	0.0180	0.0034					3.30
52	0.5164	0.1025	0.806	7.68	0.896	0.1858E+02	
52	0.0193	0.0039					5.99
53	0.4945	0.1018	0.782	7.50	0.915	0.5833E+02	
53	0.0174	0.0038					8.12
54	0.5045	0.0963	0.837	7.87	0.936	0.1010E-04	
54	0.0185	0.0035					3.87
55	0.5063	0.1176	0.709	6.92	0.770	0.1640E+04	
55	0.0183	0.0051					16.27
56	0.5389	0.1075	0.800	7.65	0.855	0.1670E+02	
56	0.0210	0.0042					6.20
57	0.5477	0.1021	0.836	7.99	0.872	0.1549E-08	
57	0.0215	0.0039					2.60
58	0.5882	0.1093	0.897	8.01	0.812	0.6075E-06	
58	0.0249	0.0044					5.39
59	0.5212	0.1210	0.912	6.92	0.838	0.5144E-03	
59	0.0196	0.0054					17.79
60	0.5439	0.0998	0.776	8.07	0.883	0.1713E+02	
60	0.0215	0.0037					0.28
61	0.5099	0.0960	0.744	7.94	0.925	0.7217E+02	
61	0.0184	0.0034					1.58
62	0.5449	0.0998	0.766	8.08	0.881	0.2254E+02	
62	0.0211	0.0037					0.00
63	0.5128	0.0940	0.861	8.08	0.938	0.3300E-05	
63	0.0188	0.0033					3.44
64	0.5045	0.0952	0.767	7.93	0.936	0.5704E+02	
64	0.0184	0.0034					2.07
65	0.5716	0.0921	0.865	8.75	0.902	0.1167E-05	
65	0.0242	0.0032					9.57
66	0.4936	0.0917	0.835	8.01	0.969	0.5575E-05	
66	0.0172	0.0032					2.40
67	0.4937	0.1030	0.770	7.43	0.910	0.6953E+02	
67	0.0170	0.0039					8.82

70	0.5162	0.0963	0.806	7.99	0.925	0.4073E+01	
70	0.0189	0.0035					1.76
71	0.4789	0.0953	0.759	7.66	0.914	0.1818E+04	
71	0.0163	0.0034					2.57
72	0.5381	0.0979	0.795	8.12	0.898	0.4733E+01	
72	0.0209	0.0035					0.06
73	0.5185	0.0958	0.767	8.04	0.921	0.3862E+02	
73	0.0191	0.0034					0.60
74	0.4771	0.1041	0.830	7.21	0.849	0.2357E+04	
74	0.0164	0.0040					10.26
76	0.5305	0.0995	0.749	7.96	0.891	0.4241E+02	
76	0.0201	0.0037					1.41
77	0.5384	0.1060	0.825	7.72	0.865	0.3058E+01	
77	0.0207	0.0043					5.68
79	0.5441	0.1083	0.755	7.66	0.843	0.3441E+02	
79	0.0214	0.0044					5.50
80	0.5849	0.1015	0.738	8.36	0.844	0.2073E+02	
80	0.0245	0.0038					4.00
81	0.5842	0.1203	0.711	7.49	0.767	0.3662E+02	
81	0.0246	0.0053					7.17
82	0.6096	0.1320	0.717	7.25	0.719	0.3100E+02	
82	0.0264	0.0064					10.59
83	0.5813	0.1404	0.683	6.73	0.715	0.4700E+02	
83	0.0241	0.0073					17.29
84	0.6163	0.1131	0.773	8.07	0.779	0.8793E+01	
84	0.0270	0.0046					0.24
85	0.6576	0.1017	0.859	8.98	0.804	0.1032E-04	
85	0.0317	0.0038					12.24
86	0.6169	0.0959	0.814	8.95	0.855	0.8504E-06	
86	0.0277	0.0034					11.17
87	0.5336	0.0995	0.764	7.99	0.891	0.3053E+02	
87	0.0202	0.0037					1.17
89	0.5811	0.0941	0.751	8.73	0.887	0.8347E+01	
89	0.0243	0.0033					8.50
90	0.5164	0.0907	0.800	8.30	0.954	0.5295E-05	
90	0.0190	0.0031					2.47
91	0.5195	0.0945	0.833	8.12	0.930	0.1225E-04	
91	0.0194	0.0033					1.89
92	0.5452	0.0932	0.842	8.44	0.915	0.5744E-05	
92	0.0209	0.0033					5.12
93	0.5437	0.0900	0.828	8.61	0.935	0.5553E-07	
93	0.0213	0.0030					7.01
94	0.5287	0.0979	0.773	8.03	0.903	0.2601E+02	
94	0.0196	0.0036					0.83
95	0.5423	0.0917	0.788	8.50	0.927	0.5593E-04	
95	0.0212	0.0031					5.15
96	0.5943	0.0965	0.809	8.71	0.865	0.2166E-05	
96	0.0251	0.0035					8.11
97	0.5415	0.0944	0.803	8.34	0.913	0.1732E-04	
97	0.0208	0.0033					3.03
98	0.5491	0.0961	0.836	8.32	0.897	0.1085E-04	
98	0.0219	0.0035					3.53
99	0.5385	0.0917	0.761	8.46	0.929	0.2017E+02	
99	0.0207	0.0031					4.99
100	0.5810	0.0972	0.761	8.56	0.870	0.7229E+01	
100	0.0246	0.0046					6.22
101	0.5282	0.0958	0.793	8.13	0.916	0.6707E+01	
101	0.0202	0.0034					0.26
102	0.5344	0.0923	0.868	8.39	0.928	0.1571E-05	
102	0.0204	0.0032					5.52

104	0.5531	0.0969	0.799	8.31	0.892	0.6100E-04	
104	0.0217	0.0035					2.62
105	0.5672	0.0944	0.852	8.58	0.893	0.3993E-05	
105	0.0226	0.0033					7.17
107	0.5885	0.1034	0.735	8.30	0.832	0.2206E+02	
107	0.0247	0.0039					3.23
108	0.5017	0.1049	0.812	7.42	0.899	0.2997E+02	
108	0.0180	0.0040					9.58
109	0.5439	0.1184	0.830	7.22	0.817	0.1436E+02	
109	0.0210	0.0053					12.51
110	0.5669	0.1315	0.664	6.92	0.743	0.5558E+02	
110	0.0228	0.0063					14.41
112	0.5298	0.1175	0.734	7.14	0.820	0.5331E+02	
112	0.0201	0.0051					12.40
113	0.5459	0.1040	0.817	7.88	0.866	0.1037E+01	
113	0.0213	0.0041					3.37
114	0.5646	0.1046	0.730	8.02	0.841	0.3358E+02	
114	0.0229	0.0041					0.29
115	0.5671	0.0976	0.831	8.40	0.877	0.1266E-05	
115	0.0230	0.0036					4.42
116	0.5367	0.0997	0.804	8.01	0.891	0.3674E+01	
116	0.0209	0.0037					1.48
118	0.5547	0.0988	0.772	8.22	0.880	0.1296E+02	
118	0.0215	0.0036					1.78
119	0.5409	0.0931	0.800	8.41	0.921	0.4763E-04	
119	0.0211	0.0032					3.92
120	0.5143	0.1038	0.898	7.59	0.894	0.1785E-04	
120	0.0189	0.0040					8.82
121	0.5234	0.0985	0.830	7.94	0.908	0.1359E-04	
121	0.0196	0.0036					2.85
122	0.5538	0.0950	0.828	8.42	0.900	0.7511E-05	
122	0.0216	0.0033					4.58
123	0.5486	0.0967	0.808	8.28	0.896	0.8766E-06	
123	0.0217	0.0034					2.30
124	0.5253	0.1095	0.741	7.44	0.852	0.5260E+02	
124	0.0198	0.0045					8.36
125	0.5305	0.1050	0.844	7.69	0.876	0.4197E-03	
125	0.0202	0.0041					6.32
126	0.5544	0.0975	0.793	8.29	0.888	0.4897E-03	
126	0.0217	0.0035					2.37
127	0.5447	0.1070	0.726	7.73	0.845	0.4589E+02	
127	0.0214	0.0043					4.20
129	0.5349	0.1315	0.541	6.65	0.692	0.1476E+04	
129	0.0203	0.0064					20.81
130	0.5613	0.1447	0.384	6.43	0.683	0.1165E+03	
130	0.0227	0.0078					17.08
131	0.6228	0.2077	0.130	5.30	0.423	0.1727E+01	
131	0.0273	0.0159					59.9
132	0.6296	0.2361	-1.292	4.80	0.289	0.4224E+03	
132	0.0284	0.0204					6.46
133	0.7454	0.3310	-5.162	4.10	0.182	0.3423E+03	
133	0.0399	0.0402					32.35
134	1.0003	0.5532	-14.305	3.18	0.097	0.2144E+03	
134	0.0717	0.1199					41.15

For each residue, the bottom row of numbers give the standard deviations of the T1 and T2 values, and the total relative deviation of theoretical values from experimental values in the fitting of order parameter and effective correlation time of internal motion.